SACADA Database Code: 228

Topology: $3,4^3T55$

# of independent nodes (IN): 4
Transitivity: [4973]
Space Group: Immm
Pearson: oI40
Coordination Number (CN): 3, 4 (1:4)

Year: 2001

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^3T55$ (SACADA #228)		2.884		1.155	301.2	259.8	40.8	SACADA[1]
bco-C20								doi: 10.1103/PhysRevB.64.245405
bco-C20								doi: 10.1140/epjb/e2003-00060-4

Elasticity tensor (kBar)[1]

5937.6346	1018.2669	1220.5108	-0.0000	0.0000	-0.0000
1018.2669	7325.7685	1043.1442	-0.0000	-0.0000	0.0000
1220.5108	1043.1442	7397.3563	0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	2023.2963	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	3251.5306	-0.0000
-0.0000	0.0000	0.0000	-0.0000	-0.0000	2171.5529

[1] We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) to calculate the total energy and properties of carbon allotropes.

DFT calculations

We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) package [6] to calculate the total energy of carbon allotropes. The Generalized Gradient Approximation [7] (GGA) for exchange-correlational functional is used everywhere. The energy cutoff set to 600 eV. Fully automatic Γ-centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025$ Å^{-1} is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10^{-6} eV for energy and 10^{-5} eV Å^{-1} for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio ν — have been calculated within the Voigt–Reuss–Hill [8] approximation. The Vicker's hardness H_v has been estimated according to Oganov's model [9].